

Hexachlorophene  
70-30-4 | DTXSID6020690

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

## Model Results

**Predicted value:**  $3.18 \times 10^{-11}$  cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Outside

**Local applicability domain index:**  $1.40 \times 10^{-1}$

**Confidence level:**  $6.34 \times 10^{-1}$

## Nearest Neighbors from the Training Set

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2-Methyl-p-benzoquinone

**Measured:**  $2.35 \times 10^{-11}$

**Predicted:**  $2.15 \times 10^{-11}$

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1,4-Naphthoquinone

**Measured:**  $3.10 \times 10^{-12}$

**Predicted:**  $3.16 \times 10^{-11}$

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1-Nitrocyclohex-1-ene

**Measured:**  $4.37 \times 10^{-11}$

**Predicted:**  $3.80 \times 10^{-11}$

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alpha-Phellandrene

**Measured:**  $3.13 \times 10^{-10}$

**Predicted:**  $2.83 \times 10^{-10}$